An Exact Dynamics of an Electron Gas at $r_s \approx 3.5$ and a Short-wavelength Limit

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ABSTRACT

We show the exact dynamic structure factor $S(k,\omega)$ of the many- electron system by calculating the relaxation function. Our $S(k,\omega)$ is asymptotically exact as $k \to \infty$ and at a particular metallic density $r_s^* \approx 3.5$. From the exact solution, we derive two static relations, $x^2 = \frac{3}{5}y$, and $x^2 = \frac{3}{16}\omega_p^2[1 - g(0)]$ valid at r_s^*, where x and y are averages of the one-particle kinetic energy and its square, respectively. Our $S(k,\omega)$ is compared with an experimental measurement for Li at $k = 2.08k_F$.

There have been many works on the many-body effects of the homogeneous electron gas with neutralizing background which is a model for simple metals. But the latter system is still not fully understandable except at the small momentum transfer and high density limit at which the random phase approximation (RPA) gives an asymptotically exact solution. For the large momentum transfer regime, on the other hand, one usually thinks of the noninteracting solution as an approximation of the interacting system. But it is not good enough, since the multi-pair excitations play an important role as momentum transfer k becomes large. The latter excitations do not appear in the noninteracting system and give rise to the high and low frequency tails in the dynamic structure factor of a large k. Therefore, the large k regime is also valuable to study many-body effects in the electron gases.

In this study, we obtain the dynamic structure factor which becomes exact at a particular metallic density $r_s \approx 3.5$, where r_s is the average distance between electrons in units of the Bohr radius, as $k \to \infty$. The method we adopt here is the recurrence relation method which gives the relaxation function in an infinite continued fraction in the Laplace transformed space.

$$\hat{\Xi}_k(z) = \frac{1}{z+} \quad \frac{\Delta_1}{z+} \quad \frac{\Delta_2}{z+} \quad \cdots(\text{continued fraction}) \tag{1}$$

The coefficients Δ_n are expressed in terms of the successive ratios of the frequency moments $c_n = (L^n\rho_k, L^n\rho_k)$, $n = 0, 1, 2\cdots$, where $L\rho_k = [H, \rho_k]$, H is the Hamiltonian. These quantities may not be obtained for the general k. But they are available in the large-k limit. The large-k expansion of the $(2n+1)$th moment c_n is written as

$$c_n = 2\sum_p \omega_p(k)^{2n-1} n_p + \frac{\rho}{(2m)^{2n-2}} \sum_q [\{ (4n-4)k^{4n-4} v_{q+k} - \frac{2}{3}(2n-1)(2n-2)(2n-3)k^{4n-8}(\vec{q}\cdot\vec{k})v_q \}\{S(q)-1\}] + (N.O.)(2)$$

where $\omega_p(k) = (k^2 + 2\vec{k}\cdot\vec{p})\hbar^2/2m$, n_p the Fermi distribution function, and $S(q)$ is the structure factor.

The successive ratio c_{n+1}/c_n is given by

$$\frac{c_{n+1}}{c_n} = P + nQ + \sum_{i=1}^{n} R_i + O(k^{-2}), \qquad n = 0, 1, 2, \cdots \tag{3}$$

where $P = k^4 - (\frac{4}{3}x)k^2 + \frac{16}{9}x^2 - \frac{16}{5}y + \frac{1}{3}\omega_p^2[1 + 2g(0)]$, $Q = (\frac{16}{3}x)k^2 - \frac{16}{9}x^2 + \frac{16}{5}y$, $R_n = -\frac{2^6}{3}(n-1)(2n-3)A - \frac{2^7}{9}(n-1)B$, where $A = x^2 - \frac{3}{5}y$, and $B = x^2 - \frac{3}{16}\omega_p^2[1 - g(0)]$. Here we denote k in units of k_F, $\hbar = 1$, ω_p the plasma frequency expressed in units of Fermi energy ϵ_F, $g(0)$ the pair correlation function at the origin, x and y are the averages of one- particle kinetic energy and its square, expressed in units of ϵ_F and ϵ_F^2, respectively.

Now let us assume that at r_s^*

$$A(r_s^*) = 0, \qquad \text{and} \qquad B(r_s^*) = 0 \tag{4}$$

This assumption will be justified later. Then we find that $\frac{c_{n+2}}{c_{n+1}} - \frac{c_{n+1}}{c_n} = Q$ at r_s^*, if we neglect $O(k^{-2})$ for a large k. Using this and retaining the consistency of neglecting $O(k^{-2})$ in c_{n+1}/c_n, the following pattern is obtained: $\Delta_{2n-1}^* = (n-1+s)Q^*$, $\Delta_{2n}^* = nQ^*$, $n = 1, 2, 3, \cdots$, where $s \equiv P^*/Q^*$ and the $*$ means the value at the density r_s^*. The dynamic structure factor $S(k,\omega)$ is related to the relaxation function by the fluctuation-dissipation theorem as

follows:

$$\tilde{S}(k,\omega) \equiv S(k,\omega)/c_0 = \frac{1}{\pi}\mathrm{Im}[z\hat{\Xi}_k(z)]_{z=-i\omega+\epsilon} \tag{5}$$

From the delta pattern shown above, we obtain the dynamic structure factor at r_s^* as[1]

$$\tilde{S}^*(k,\omega) = \frac{\omega^{2s}}{Q^{*s}\Gamma(s)}e^{-\omega^2/Q^*} \tag{6}$$

where ω is expressed in units of ϵ_F. Thus (6) is an asymptotically exact dynamic structure factor of the electron gas at r_s^* under the assumption (4).

Now we justify the assumption. The process is composed of two parts. First we derive $A^* = 0$ and then derive $A^* = \alpha B^*$, where α is a constant. For the first, we use a relation which may be called the one-particle kinetic energy sum rule valid at large-k limit.[2] It is given at zero temperature as follows:

$$\langle T^n\rangle = \lim_{k\to\infty}\frac{2n+1}{(4\omega_r)^n}\int_0^\infty S(k,\omega)(\omega-\omega_r)^{2n}d\omega, \quad n=1,2,\cdots \tag{7}$$

where ω_r is the frequency at which $(\partial/\partial\omega)S^*(k,\omega) = 0$. Substituting (6) into (7) with $\omega_r = (sQ^*)^{\frac{1}{2}}$, we obtain, for $n=2$, $\langle T^2\rangle^* = \frac{5}{3}x^{*2} = y^*$, where we use the definition $\langle T^2\rangle = y$. This justifies the first part, $A^* = 0$, of the assumption. For the second part, the Kimball's relation[3] $\frac{1}{2}\omega_p^2 g(0) = \lim_{k\to\infty}\{k^4[1-S(k)]\}$ has been used. Using the large-k expansion of the structure factor $S^*(k)$ obtained by integrating (6) for ω, we obtain the relation $B^* = x^{*2} - \frac{3}{16}\omega_p^{*2}[1-g^*(0)] = \frac{9}{4}A^*$. Hence, with the first derivation $A^* = 0$, we get $B^* = 0$. Thus (4) is justified.

It is interesting to find the value of r_s^*. Lantto, Pietilainen, and Kallio[4] obtained $n(k)$, x, and $g(0)$ through a Jastrow variational method and Lantto

calculated y in terms of their $n(k)$. Lantto's data for the latter three quantities are the only available data obtained simultaneously by one method as far as we know. Shown in Fig. 1 is A and B vs r_s plotted on the basis of the data given by Lantto. We observe that A and B vanish simultaneously at $r_s^* \approx 3.5$ which is close to the density of Li for which an experimental data for $S(k,\omega)$ at $k = 2.08k_F$ has been given. We compare the theoretical dynamic structure factor (6) for $k = 2.08$ with experiment in Fig. 2. Also shown is the RPA result at the same value of k. Since the RPA and the ideal dynamic structure factors do not have the tails, they cannot explain the large-k property of the system appropriately.

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References

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Fig. 1

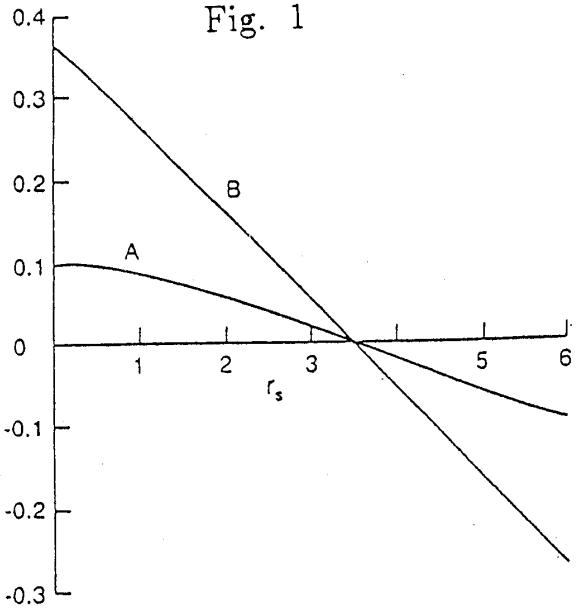

Fig. 2